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Lyapunov exponents from quantum dynamics

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Abstract. We extract classical Lyapunov exponents from the time dependence of quantum mechanical expectation values. Classical chaos is revealed as a quantum transient with a liftetime $\sim \ln \hbar$. Our strategy is shown to work for the example of a periodically kicked top.

Keywords: Theory and models of chaotic systems; Quantum mechanics; Foundations.

1 Introduction

Solving Schrödinger's equation in semiclassical approximations is a highly developed art for classically integrable systems, but the object of ongoing research for classically chaotic situations [1]. Reverting the usual perspective [2], we here propose to investigate how well certain properties of classical dynamics are reflected in quantum mechanics [3, 4]. Our aim is to tell apart regular and chaotic classical motion by inspecting the time evolution of the quantum system. Moreover, we want to elucidate the emergence of classical chaos in quantum dynamics as the classical limit is approached. More specifically, we shall extract the Lyapunov exponent from the time dependence of quantum mechanical expectation values. We shall also compare our approach with related work [3, 4].

2 The Lyapunov exponent for quantum dynamics

At the basis of our study lies a generalization of the Lyapunov exponent,

$$\lambda = \lim_{t\to\infty} \lambda(t), \quad \lambda(t) = \lim_{d(0)\to 0} \frac{1}{t} \ln\left(\frac{d(t)}{d(0)}\right), \tag{1}$$

where $d(t)$ is a distance between two states at time t; the states in question must be chosen in close mutual proximity initially such that the time evolution of the difference vector is linear up to time t. In classical mechanics, $d(t)$ may be specified as the Euclidian distance between two phase space points. A positive value of λ implies exponential separation in time of trajectories and thus chaos. Regular motion, on the other hand, is characterized by $\lambda \leq 0$.

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The pursuit of our goal requires to replace the classical distance in (1) by one of quantum mechanical legitimacy [3, 4]. To that end we employ, for a system with f degrees of freedom, the $2f$-tuple of position and momentum operators $\mathbf{X}$ and two wave vectors $\psi_i(t)$, $i = 1, 2$, to define

$$d = |\langle\psi_1(t)|\mathbf{X}|\psi_1(t)\rangle - \langle\psi_2(t)|\mathbf{X}|\psi_2(t)\rangle| . \tag{2}$$

Even though this notion of a distance will turn out to work well we should note that it does not constitute a metric in Hilbert space because different states ψ may have the same expectation value $\langle\psi|\mathbf{X}|\psi\rangle$. In order to make sure that the distance (2) takes on the familiar meaning in the classical limit we shall restrict ourselves to coherent initial states $\psi_{1,2}(0)$. Such states have the minimum uncertainty product allowed by the uncertainty principle, $\delta^{2f}X = \delta^f p \delta^f x \sim \hbar^f$. Of course, an initially coherent state will not in general remain coherent for $t > 0$. We shall therefore have to find out how long in time an expectation value $\langle\psi(t)|\mathbf{X}|\psi(t)\rangle$ can remain reasonably faithful to classical dynamics.

3 Semiclassical considerations

Quantum fluctuations degrade the reliability of the quantum "prediction" for a classical trajectory both through the initial spread $\delta^{2f}X$ in $\psi(0)$ and through the unitary time evolution of $\psi(t)$. For a crude measure of such degrading a hybrid description may be employed: One allows for classical dynamics but retains the initial spread $\delta^{2f}X$. A coherent initial state is thus represented by a cloud of phase space points located in a region of size $\hbar^f$ around the point specified by $\langle\psi(0)|\mathbf{X}|\psi(0)\rangle$. A bundle of trajectories originates from that cloud, and the divergence of the bundle will characterize the degrading in question. The maximum distance between any two points of the moving cloud will grow exponentially, $|\delta\mathbf{X}(t)| \sim \sqrt{\hbar}e^{\lambda t}$, for chaotic motion. This reasoning suggests that quantum mechanics cannot yield reliable predictions of classically chaotic motion for times exceeding

$$\tau \sim (1/\lambda) \ln (S/\hbar) \tag{3}$$

where S is an action typical for the classical motion [4–8]. Loosely speaking, classical chaos is accomodated in quantum mechanics as a transient with lifetime τ. As is well known, for times $t \gg \tau$ the behavior of quantum means is quasiperiodic, at least for systems with discrete (quasi-)energy spectra.

The foregoing estimate of the lifetime of chaos poses a dilemma for any attempt at determining a Lyapunov exponent from quantum data. While the definition (1) involves an infinite-time limit, the quantum distance (2) will grossly deviate from its classical counterpart at times $t > \tau$. Of course, in actual numerical work one increases t only until $\lambda(t)$ attains a stationary value. When employing the quantum distance (2) the question arises whether $\lambda(t)$ reaches its classical "plateau" for $t < \tau$, i.e. before chaos is bound to die and $\lambda(t)$ thus decays to zero. When the time of saturation of $\lambda(t)$ is known from a classical analysis of a specific system, one can use the lifetime (3) to estimate a critical value of $\hbar/S$. For $\hbar/S$ below the critical value it should be possible to determine the Lyapunov exponent from quantum mechanics. As we shall show below, computers presently available begin to allow for such a program.

4 The kicked top as a model

We now turn to the study of a model system, a periodically kicked top [2, 9–12]. Its dynamical variables, the three components of an angular momentum, have the commutators $[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k$. For a period-to-period stroboscopic description we employ the Floquet operator

$$F = \exp(-ikJ_x^2/2\hbar^2 j)\exp(-i\pi J_z/2\hbar)\,. \tag{4}$$

The evolution of the state vector may then be written as the quantum map $\psi(t+1) = F\psi(t)$, where the dimensionless discrete time t counts the number of periods passed. The dynamics conserves the squared angular momentum, $\mathbf{J}^2 = \hbar^2 j(j+1)$. Once the quantum number j is fixed the Floquet operator can be represented by a $(2j+1)\times(2j+1)$ matrix. Moreover, j controls the weight of quantum fluctuations as $S \sim j$, i.e. $\hbar \sim 1/j$ and yields the lifetime τ according to (3) as $\tau \sim (1/\lambda)\ln j$. Especially, the classical limit is attained as $j \to \infty$.

The classical phase space, the sphere $\mathbf{J}^2/\hbar^2 j^2 = 1$, is conveniently parametrized by two angles, $\phi \in [0, 2\pi)$ and $\theta \in [0, \pi]$. The stroboscopic dynamics takes the form of a map $(\phi_t, \theta_t) \to (\phi_{t+1}, \theta_{t+1})$. While for $k = 0$ that map describes a rotation around the axis $\theta = 0$ by $\pi/2$ and thus is integrable, chaos arises for larger values of the kicking strength k. In our numerical work we have set $k = 3$, at which value the phase space is dominated by chaos but still has sizeable regular islands as can be seen in Fig. 1. The variation of the classical Lyapunov exponent along the meridian ($\phi = 3\pi/4$; $0 \le \theta \le \pi$), displayed in Fig. 2, reveals a large island of stability in $0.6 \le \theta \le 1.4$ and four smaller ones at $\theta \approx 0.55, 1.53, 2.67$ and 2.74. In calculating the Lyapunov exponent as a function of θ for Fig. 2a, we have employed $\lambda(t)$ according to (1) with the Euclidian distance $d(t) = |\mathbf{J}_1(t) - \mathbf{J}_2(t)|$, restricting t to 10^5 iterations. Note from Fig. 2a that λ appears constant throughout the chaotic ranges; five "holes" with $\lambda = 0$ correspond to the regular islands mentioned.

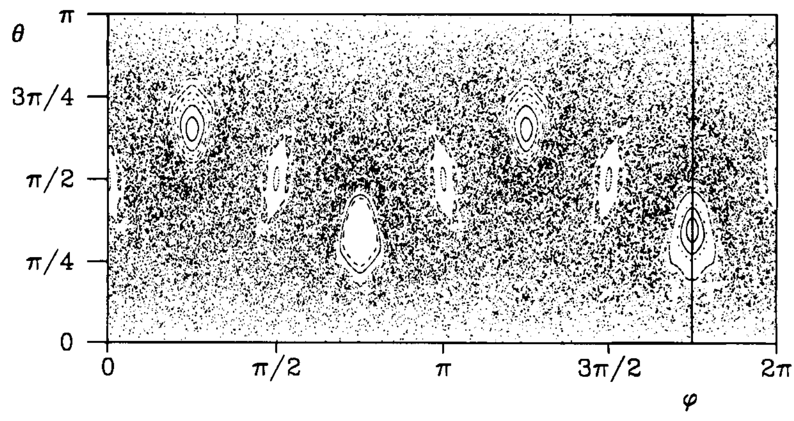

Fig. 1 The classical phase space portrait of the kicked top for $k = 3$. The straight line indicates the cross section along which the Lyapunov exponent is calculated.

In order to find the smallest time t allowing to estimate λ we have computed $\lambda(t)$ from the classical map as a function of t for two points on the meridian mentioned, one in a regular island ($\theta = 1.0$) and the other in the chaotic range ($\theta = 2.0$). As is obvious from

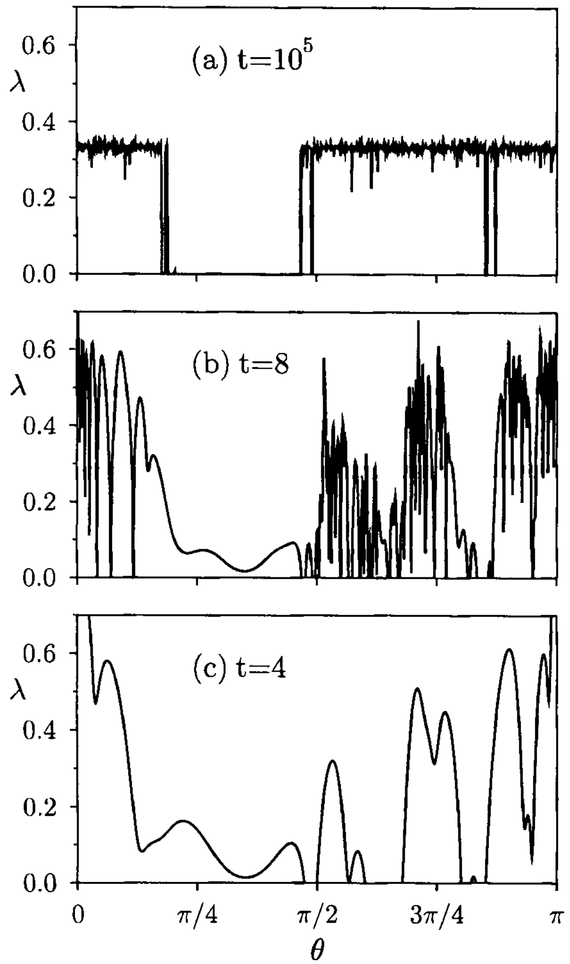

Fig. 2 The classical Lyapunov exponent λ on the cross section of the classical phase space as a function of the angle ϑ. The number of iterations t is equal to: **(a)** 100000 (asymptotic limit); **(b)** 8; **(c)** 4.

Fig. 3, $\lambda(t)$ stabilizes more rapidly for regular motion ($\lambda(t) \to 0$) than for chaos. In the latter case, accepting an uncertainty of, say, 10% for λ one may even restrict t to about 20 iterations. In anticipation of the quantum calculations, we may obtain a crude estimate of the minimum dimension $(2j + 1)$ of the Floquet matrix F by requiring $\tau = (1/\lambda) \ln j > 20$; by taking $\lambda \approx 0.33$ from Fig. 2a we have $j > 700$. But of course this is only a crude estimate of the required j.

A glance back at Fig. 2 is now indicated; parts (b) and (c) depict the variation of $\lambda(t, \theta)$ along the same meridian as part (a) but the number of iterations t is 8 for (b) and as small as 4 for (c). As must be expected, the fluctuations displayed by λ as θ varies have amplitudes decreasing with growing t. Interestingly, already for $t = 4$ the main island of stability is detectable in $\lambda(4, \theta)$. For $t = 8$ an average of $\lambda(8, \theta)$ over the chaotic range roughly equals the asymptotic long-time result, $\lambda(\infty, \theta) = 0.33$.

An aside on the temporal fluctuations of $\lambda(t)$ may be in order. According to (1) we can write $\lambda(t) = (1/t) \sum_{m=1}^{t} \ln[d(t)/d(t-1)]$, such that $\lambda(t)$ appears as the temporal mean of "single-step exponents". Since $d(t)$ varies quite erratically in each iteration for classical motion, so will the single-step exponent. If each iteration contributed independently one would expect the relative fluctuations of the sum $\lambda(t)$ to decay as $1/\sqrt{(t)}$.

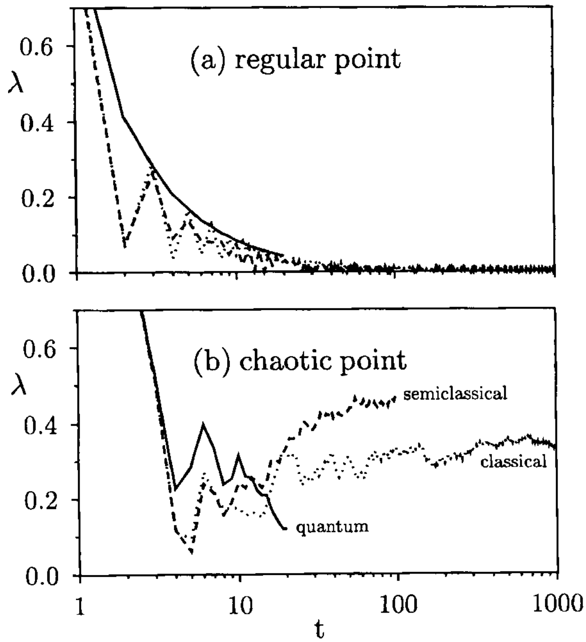

Fig. 3 Lyapunov exponent λ calculated as a function of time: **(a)** for a classically regular point ($\theta = 1.0$) and **(b)** for a chaotic one ($\theta = 2.0$). (The dotted line is for the classical case, the dashed line for a classical cloud representing a coherent state for $j = 2000$ and the straight line for the quantum mechanical case.)

Before embarking on our quantum mechanical calculation it is well to undertake one more preparatory exploration. As already mentioned a coherent quantum state defines a phase space vector only to within a finite uncertainty $\delta^{2f}X \approx \hbar^f$. In the case of our top this uncertainty amounts to an angular aperture $\delta\Omega = \sin\theta\delta\theta\delta\phi \approx 2\pi/j$. Returning to the hybrid description already used above we consider two bundles of classical trajectories. Each bundle originates from a cloud of 10^3 points which simulates, in its location and spread, a coherent state with $j = 2000$. By using the Euclidian distance between the expectation value $\langle \mathbf{j} \rangle / |\langle \mathbf{j} \rangle|$ we have once more determined $\lambda(t)$. The results thus obtained are depicted as the dashed curves in Fig. 3. As for the curves based on individual trajectories, after but a few iterations of the classical map regular and chaotic motion can be told apart.

We finally proceed to the quantum dynamics of the kicked top. Fig. 4 is meant to give an impression of how the unitary evolution changes when the classical dynamics is turned from regular to chaotic. We display the corresponding Husimi functions $Q(\theta, \phi, t) = (1/\pi) |\langle \theta, \phi | \psi(t) \rangle|^2$ where $|\psi(t)\rangle$ denotes the time dependent state vector and $|\theta, \phi\rangle$ the coherent state assigning the direction θ, ϕ with the precision $\sin\theta\delta\theta\delta\phi \sim 1/j$ to the angular momentum. If the initial state $|\psi(0)\rangle$ is taken to be a coherent state $|\theta_0, \phi_0\rangle$ residing within an island of classically regular motion, the Husimi funtion remains well localized within that island and approximately retains a Gaussian form. If, however, $|\psi(0)\rangle = |\theta_0, \phi_0\rangle$ is located anywhere in the domain of classical chaos, $Q(\theta, \phi, t)$ rapidly spreads out over the whole domain and assumes a rather erratic multipeaked appearance. The latter behavior again illustrates the dilemma mentioned in Sec. 3: To obtain a well stabilized Lyapunov exponent $\lambda(t)$ one needs to follow the evolution for long times; on the other hand, at large times the state $|\psi(t)\rangle$ tends to delocalize and thus can hardly be well represented by the expectation value $\langle \psi(t) | \mathbf{J} | \psi(t) \rangle$ in (2).

The quantum versions of $\lambda(t)$, based on the definitions (1, 2) with $|\psi_{1,2}(t)\rangle = F^t |\psi_{1,2}(0)\rangle$ and the Floquet matrix (4) for $k = 3$ and $j = 2000$, are depicted as the full curves in Fig. 3. Even in the chaotic case, $\lambda(t)$ tends to zero for $t > \tau$, i.e. as the state

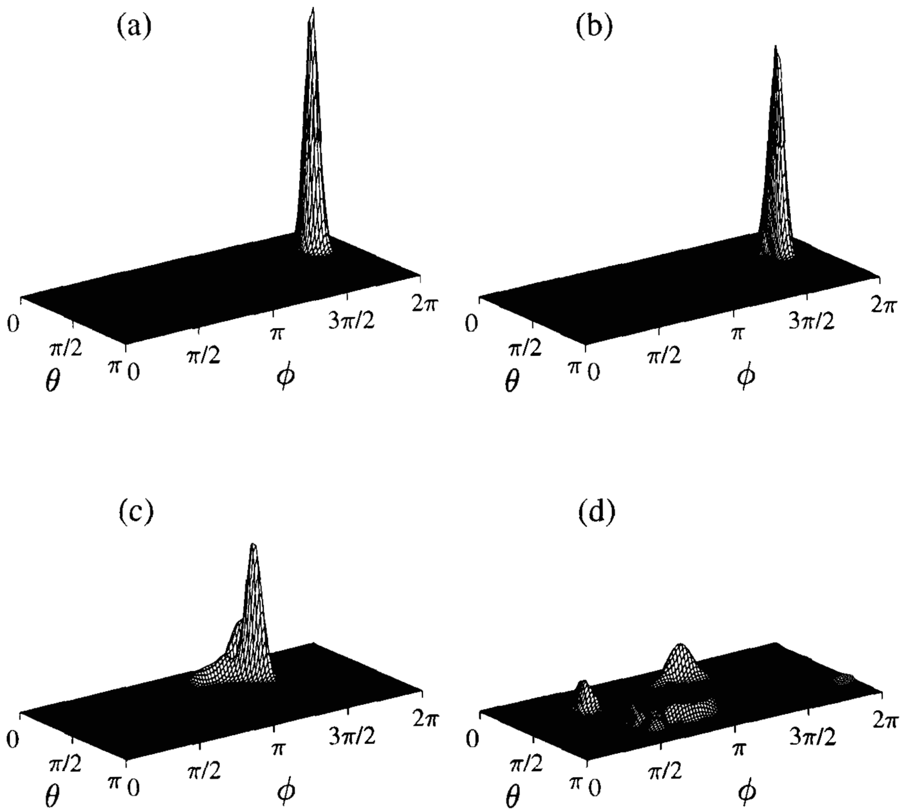

Fig. 4 Husimi distribution evolving from initially coherent states. In **(a)** and **(b)** the distributions after 4 and 10 iterations are depicted for an initial state within the regular island. In **(c)** and **(d)** the corresponding distributions for an initial state in the chaotic region illustrate the spread over the whole region.

$|\psi(t)\rangle$ begins to cover the whole classical chaotic range and the dynamics becomes manifestly quasiperiodic. In order to find the optimal escape from the dilemma for the number t of iterations we have minimized as

$$\int_0^\pi d\theta \{\lambda_{\rm class}(\theta, \infty) - \lambda_{\rm qm}(\theta, t)\}^2 = \min . \tag{5}$$

This criterion leads to $t = 4$ for $k = 3, j = 100$ and to $t = 8$ for $k = 3, j = 2000$. Fig. 5 displays these quantum mechanical Lyapunov exponents in their dependence on θ.

One may expect the optical time span t and the realiability of $\lambda(\theta, t)$ to grow as j is increased. Unfortunately, the logarithmic dependence on j of the estimate (3) of the life time τ of classical chaos as a quantum transient reflects a serious obstacle to practical calculations. For a substantial improvement of $\lambda(\theta, t)$ the optimal number of iterations t might have to be doubled or tripled; the corresponding increase of j would make for an unreasonable demand on presently available computers. It is fair to conclude, though, that the results displayed in Fig. 5 begin to ascertain classical chaos as a quantum transient.

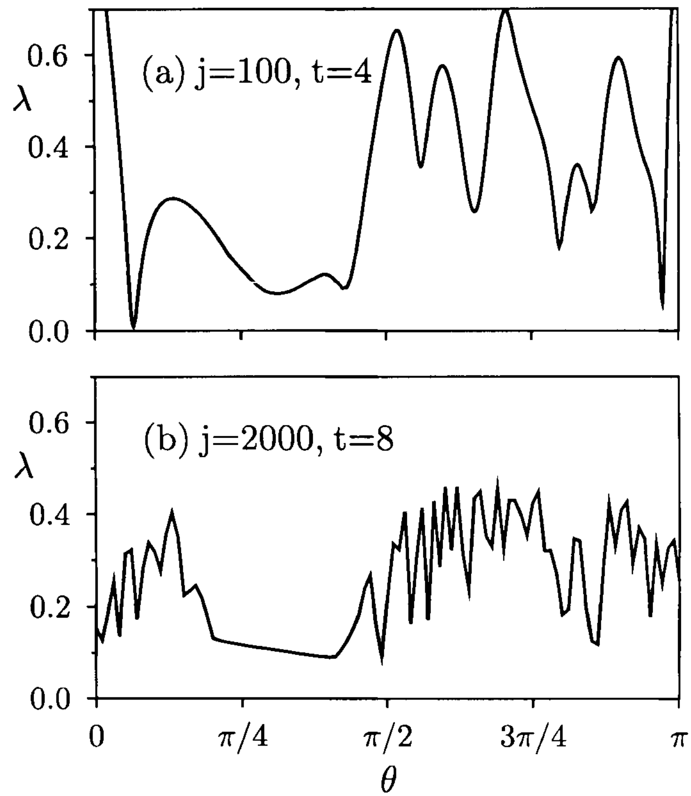

Fig. 5 Lyapunov exponent λ from quantum mechanical expectation values; (a) $j = 100$, $t = 4$; (b) $j = 2000$, $t = 8$.

Summary and comparison with related work

We have explored a strategy to extract the classical Lyapunov exponent from quantum dynamics. Instead of the classical distance between phase space points we employ a distance between expectation values of quantum observables, evaluated for two states originating from neighbouring coherent initial states. Just like in the familiar classical case the exponent is obtained after taking two separate limits, one requiring large times and the other a small initial distance. In going to large times a serious obstacle is encountered: the quantum time evolution cannot be faithful to classically chaotic behavior for times exceeding $\tau \sim \ln(1/\hbar)$, the life time of chaos as a quantum transient. With presently available computers the latter obstacle prevents us from recovering the classical exponent with good precision. The attained accuracy suffices, however, to tell apart regular and chaotic motion.

Our work is similar in spirit to that of Toda and Ikeda [3]. These authors determine a Lyapunov exponent by following the quantum evolution of a single initial state, rather than a distance between two states. They measure the temporal growth of the length of a typical contour line of the Husimi distribution. Our definition (1,2) is more closely analogous to the classical one; especially, the possibility to implement the limit $d(0) \to 0$ by the zigzag procedure described in the Appendix seems to offer technical advantages.

The double limit $d(0) \to 0$ and $t \to \infty$ is also inherent in the work of Frahm and Mikeska [4] on a periodically driven top. Since that investigation is based on an approximate semiclassical solution of Schrödinger's equation, there is no upper but in fact a lower bound to the quantum number j; the authors estimate $j \geq 10^6$ as a condition for their Gaussian ansatz for the state $|\psi(t)\rangle$ to remain valid up to times at which $\lambda(t)$ stabilizes. Clearly, Ref.[4] and the present paper are complementary in their specific strength and weakness.

Appendix: Classical and quantum "zigzags"

We would like to add some remarks of a slightly technical nature. In order to perform the double limit $t \to \infty$ and $d(0) \to 0$ in (1) it is convenient to employ the following "zigzag" procedure [13]: In classical work, one chooses a reference point $\mathbf{X}_1(0)$ and a satellite $\mathbf{X}_2(0)$ with a small but finite distance $d(0) = |\mathbf{X}_1(0) - \mathbf{X}_2(0)| \equiv |\mathbf{X}_{12}(0)|$. The evolution of $d(t)$ is followed for a finite time interval Δt, such that the difference vector $\mathbf{X}_{12}(t)$ remains a linear perturbation of $\mathbf{X}_1(t)$ for times $0 \leq t \leq \Delta t$. One then sets a new initial condition by shifting the satellite point $\mathbf{X}_2(\Delta t)$ to $\mathbf{X}_2'(\Delta t) = \mathbf{X}_1(\Delta t) + \mathbf{X}_{12}(\Delta t) d(0)/d(\Delta t)$. The distance $|\mathbf{X}_1 - \mathbf{X}_2'|$ is thus rescaled to the original value $d(0)$. Since linear dynamics of $\mathbf{X}_{12}(t)$ is secured, $\mathbf{X}_2'(\Delta t)$ is the point the satellite trajectory would have reached after the time Δt from a starting point $\mathbf{X}_2'(0) = \mathbf{X}_1(0) + \mathbf{X}_{12}(0) d(0)/d(\Delta t)$. When this procedure is iterated many times one implicitly implements the double limit in question without having to deal with inconveniently small numerical values for the distance. Moreover, when determining $\lambda(t)$ from a relatively small number of iterations t, it is necessary to employ several satellite points and to settle on the one yielding the largest $\lambda(t)$.

We have found it useful to adapt the zigzag procedure to the quantum case. After choosing a coherent state $\psi_1(0)$ and a coherent companion $\psi_2(0)$ and following their stroboscopic evolution up to some Δt we must shift the companion $\psi_2(\Delta t) = F^{\Delta t}\psi_2(0)$ to some $\psi_2'(\Delta t)$ so as to rescale the distance according to (2) back to the original one, $d(\psi(\Delta t), \psi_2'(\Delta t)) = d(\psi_1(0), \psi_2(0))$. To construct a useful $\psi_2'(\Delta t)$ we recall from [13–15] that the coherent states of angular momenta can be labeled by the complex number $\alpha = (\theta/2)e^{i\phi}$. The physical meaning of α is not of relevance here, save for the fact that neighbouring points in the α plane label coherent states with a small distance (2): Writing $\phi(\alpha)$ for a coherent state we have $d(\phi(\alpha), \phi(\alpha + \Delta\alpha)) \sim \Delta\alpha$ for $\Delta\alpha \to 0$. We assume $\psi_1(0) = \phi(\alpha)$ and $\psi_2(0) = \phi(\alpha + \Delta\alpha) = \phi(\alpha) + \Delta\alpha d\phi/d\alpha$ and define the shifted companion as $\psi_2'(\Delta t) = F^{\Delta t}\phi(\alpha + \beta\Delta\alpha) = \psi_1(\Delta t) + \beta(\psi_2(\Delta t) - \psi_1(\Delta t))$. By choosing $\beta = d(\psi_1(0), \psi_2(0))/d(\psi_1(\Delta t), \psi_2(\Delta t))$ we achieve the desired rescaling to within corrections of order $(\delta\alpha)^2$. For the sake of clarity we should add that the reference state $\psi_1(\Delta t)$ as well as the companion states $\psi_2(\Delta t)$ and $\psi_2'(\Delta t)$ do not remain coherent states for $\Delta t = 1, 2, 3 \ldots$ (see again Fig. 4).

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